WHY DO WE NEED DEEP GENERATIVE MODELING?

Jakub M. Tomczak

13 January 2020

VRIJE UNIVERSITEIT AMSTERDAM

Introduction

IS GENERATIVE MODELING IMPORTANT?

We learn a neural network to classify images:

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p(**panda**|x)=0.99

...

IS GENERATIVE MODELING IMPORTANT?

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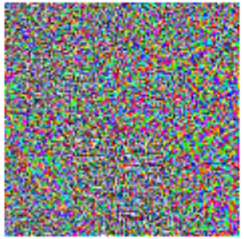
+



=

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noise

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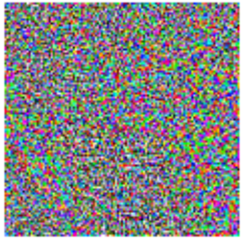

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IS GENERATIVE MODELING IMPORTANT?

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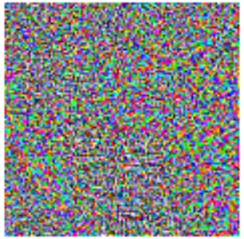

=

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...

noise

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...
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There is no semantic understanding of images.

IS GENERATIVE MODELING IMPORTANT?

This simple example shows that:

- A discriminative model is (probably) **not enough**.
- We need a notion of **uncertainty**.
- We need to **understand** the reality.

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A possible solution is **generative modeling**.

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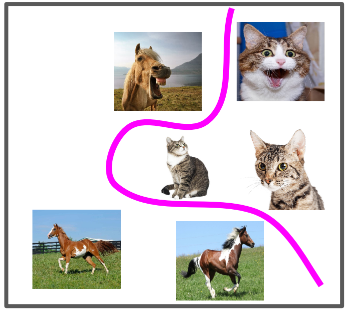
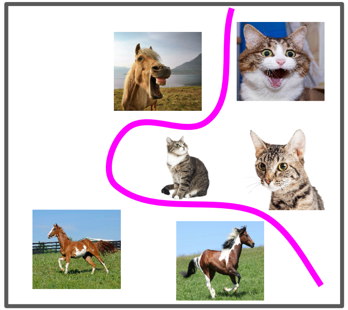


$$p_\theta(y|x)$$

IS GENERATIVE MODELING IMPORTANT?



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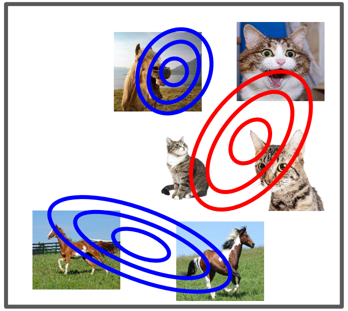

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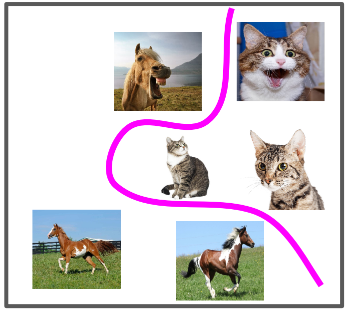

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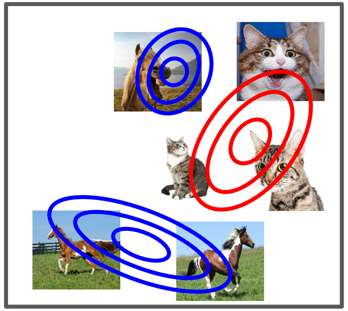

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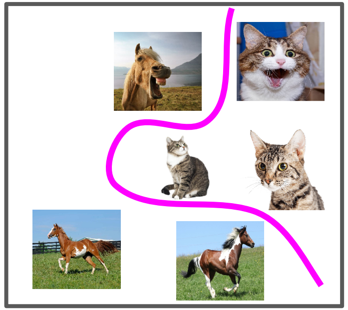
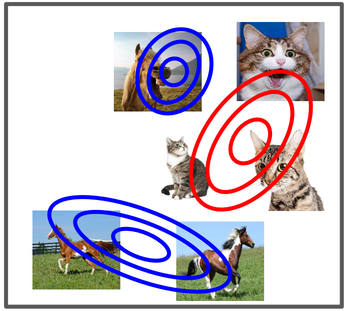


$$p_\theta(y|x)$$

High probability of a **horse.**

=

Highly probable decision!



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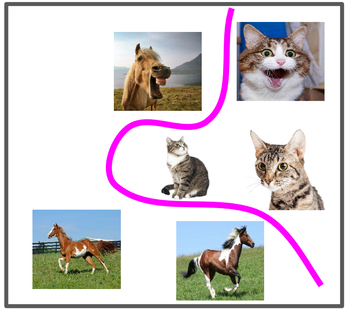

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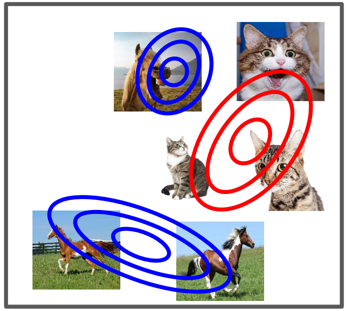

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High probability of a **horse.**
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Low probability of the **object**
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Uncertain decision!

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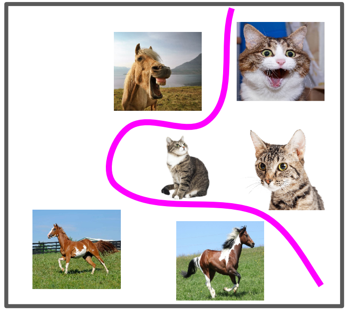

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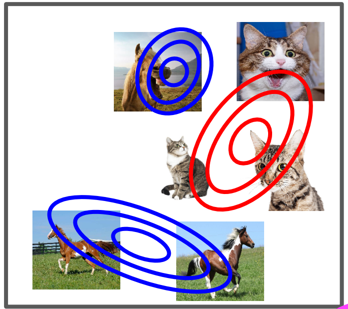

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!

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Uncertain decision!

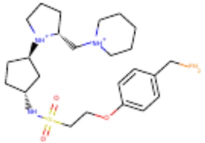
WHERE DO WE USE DEEP GENERATIVE MODELING?

" i want to talk to you . "
"i want to be with you . "
"i do n't want to be with you . "
i do n't want to be with you .
she did n't want to be with him .

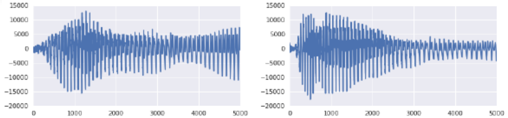
he was silent for a long moment .
he was silent for a moment .
it was quiet for a moment .
it was dark and cold .
there was a pause .
it was my turn .

Text analysis

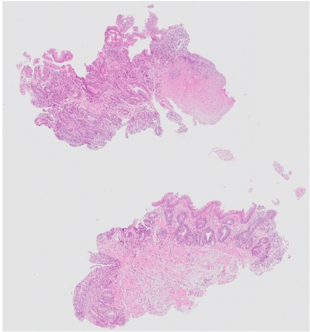
Image analysis



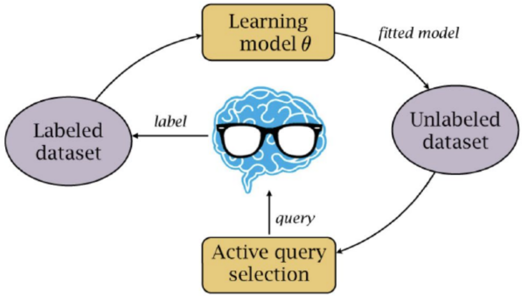
Graph analysis



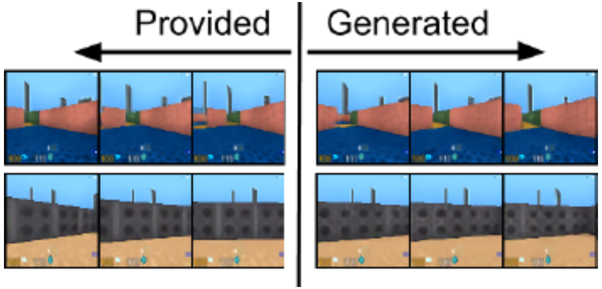
Audio analysis



Medical data



Active Learning



Reinforcement Learning

and more...

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HOW TO FORMULATE GENERATIVE MODELS?

Generative model

- **Autoregressive (*e.g.*, PixelCNN)**
- **Flow-based (e.g., RealNVP, GLOW)**
- **Latent variable models**
  - **Implicit models (*e.g.*, GANs)**
  - **Prescribed models (*e.g.*, VAE)**

HOW TO FORMULATE GENERATIVE MODELS?

	Training	Likelihood	Sampling	Compression
Autoregressive models (e.g., PixelCNN)	Stable	Exact	Slow	No
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flow-based models

GENERATIVE MODELS AS (SPHERICAL) COWS

flow-based models

latent variable models

Deep latent variable models

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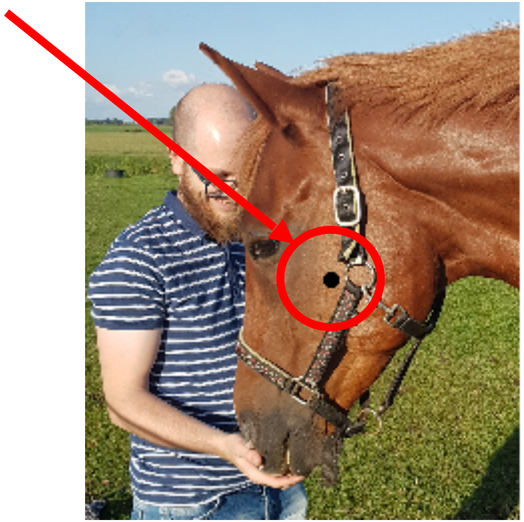

GENERATIVE MODELING

Modeling in high-dimensional spaces is difficult.

Modeling **all dependencies** among pixels:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{c=1}^{C} \psi_c(\mathbf{x}_c)$$

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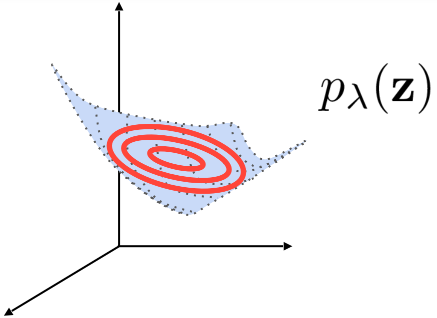
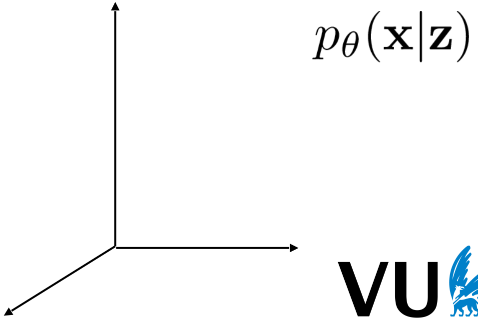
A possible **solution**: **Latent Variable Models**!

GENERATIVE MODELING WITH LATENT VARIABLES

Generative process:

1. $\mathbf{z} \sim p_\lambda(\mathbf{z})$
2. $\mathbf{x} \sim p_\theta(\mathbf{x}|\mathbf{z})$





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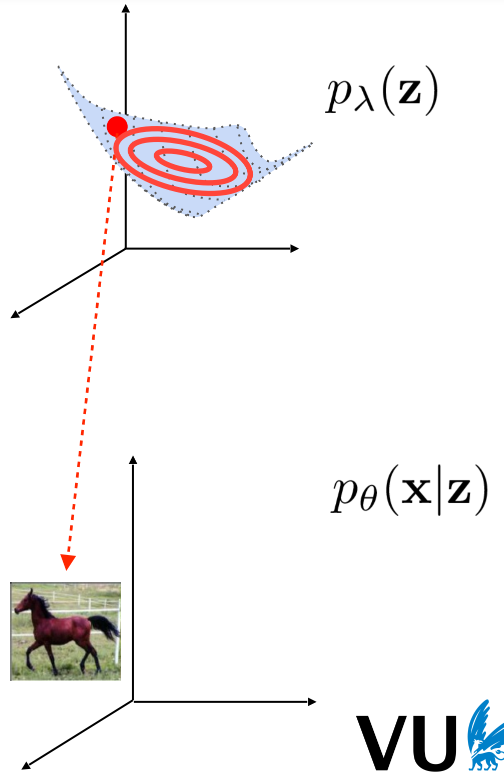

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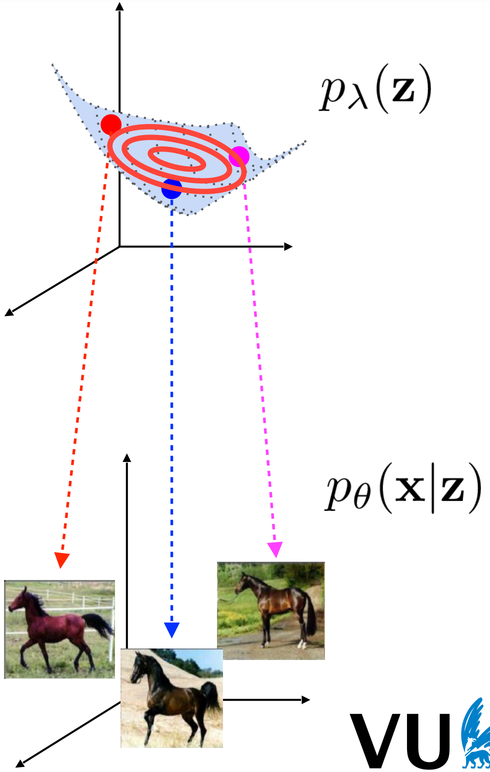

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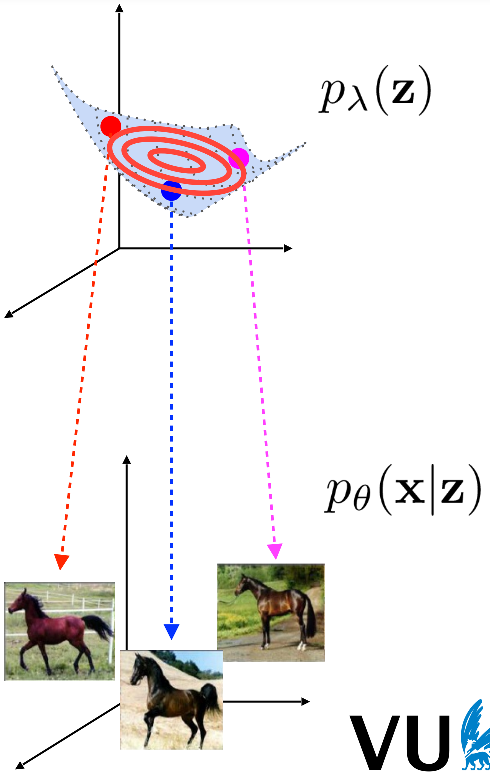
Log of marginal distribution:

$$\log p_{\vartheta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})\mathrm{d}\mathbf{z}$$



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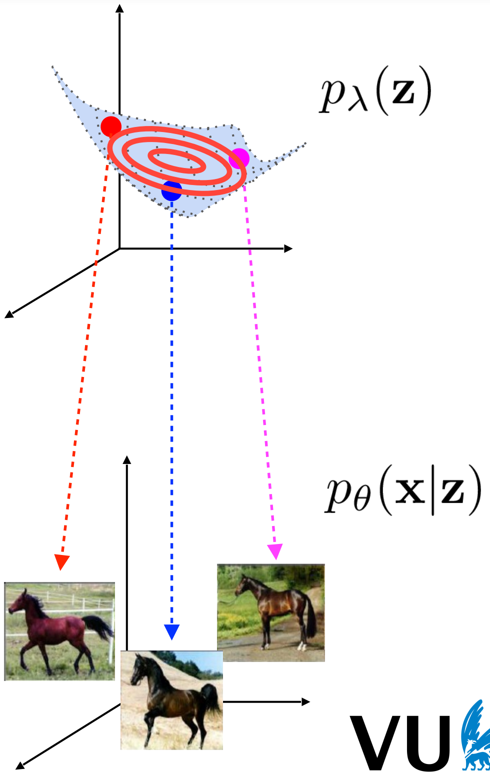
How to train such model efficiently?



VARIATIONAL INFERENCE FOR LATENT VARIABLE MODELS

$$
\begin{aligned}
\log p_\vartheta(\mathbf{x}) &= \log \int p_\theta(\mathbf{x}|\mathbf{z})\ p_\lambda(\mathbf{z})d\mathbf{z} \\
&= \log \int \frac{q_\phi(\mathbf{z}|\mathbf{x})}{q_\phi(\mathbf{z}|\mathbf{x})} p_\theta(\mathbf{x}|\mathbf{z})\ p_\lambda(\mathbf{z})d\mathbf{z} \\
&\geq \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x}|\mathbf{z})\ p_\lambda(\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})} d\mathbf{z} \\
&= \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\Big[\log p_\theta(\mathbf{x}|\mathbf{z})\Big] - \mathrm{KL}\Big(q_\phi(\mathbf{z}|\mathbf{x}) || p_\lambda(\mathbf{z})\Big)
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Variational posterior

VARIATIONAL INFERENCE FOR LATENT VARIABLE MODELS

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Jensen's inequality

$$\geq \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})}{q_{\phi}(\mathbf{z}|\mathbf{x})} \mathrm{d}\mathbf{z}$$

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&= \underbrace{\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}\Big[\log p_{\theta}(\mathbf{x}|\mathbf{z})\Big]}_{\text{Reconstruction error}} - \underbrace{\mathrm{KL}\Big(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\lambda}(\mathbf{z})\Big)}_{\text{Regularization}}
\end{aligned}
$$

VARIATIONAL INFERENCE FOR LATENT VARIABLE MODELS

decoder

encoder

marginal

$$
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decoder

encoder

marginal

= Variational Auto-Encoder

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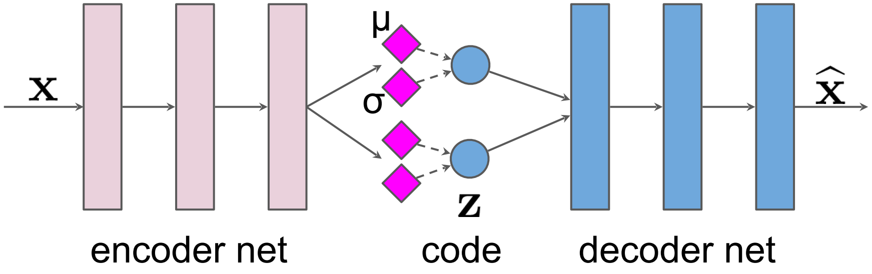
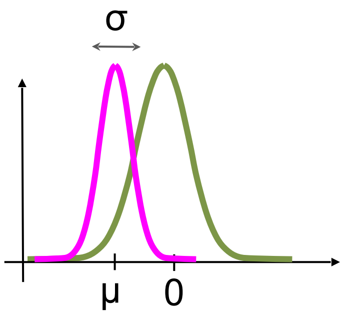
VARIATIONAL AUTO-ENCODERS

Variational posterior (**encoder**) and likelihood function (**decoder**) are parameterized by neural networks.

Reparameterization trick: move the stochasticity to independent random variables



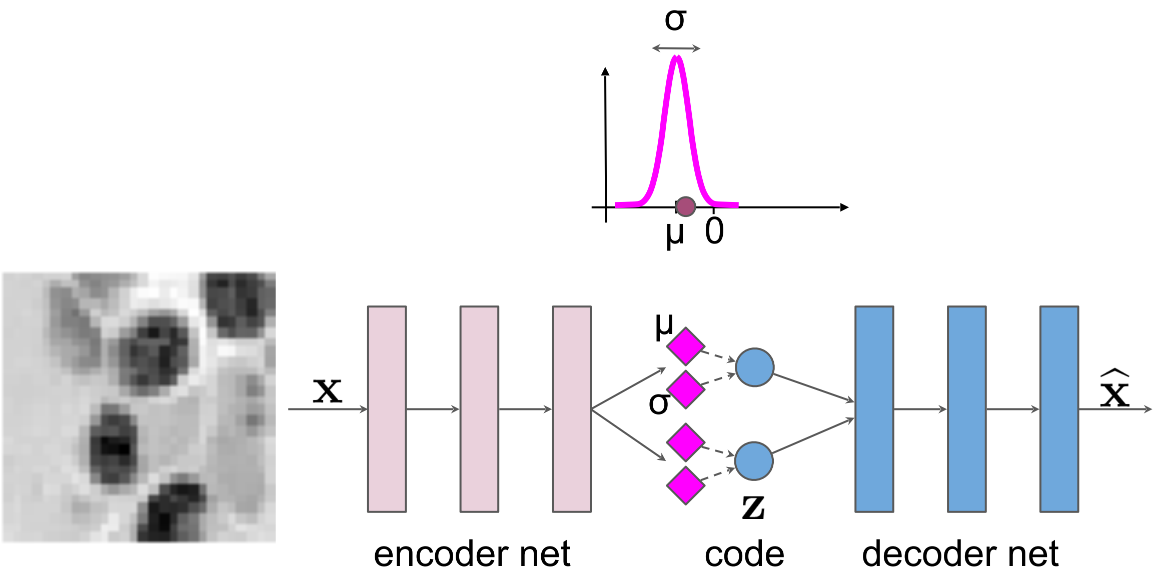
$$\mathbf{z} = f(\boldsymbol{\mu}, \boldsymbol{\sigma}; \boldsymbol{\varepsilon}), \text{ where } \boldsymbol{\varepsilon} \sim p(\boldsymbol{\varepsilon})$$



VARIATIONAL AUTO-ENCODERS

VAE copies input to output through a **bottleneck**.

VAE learns a **code** of the data.



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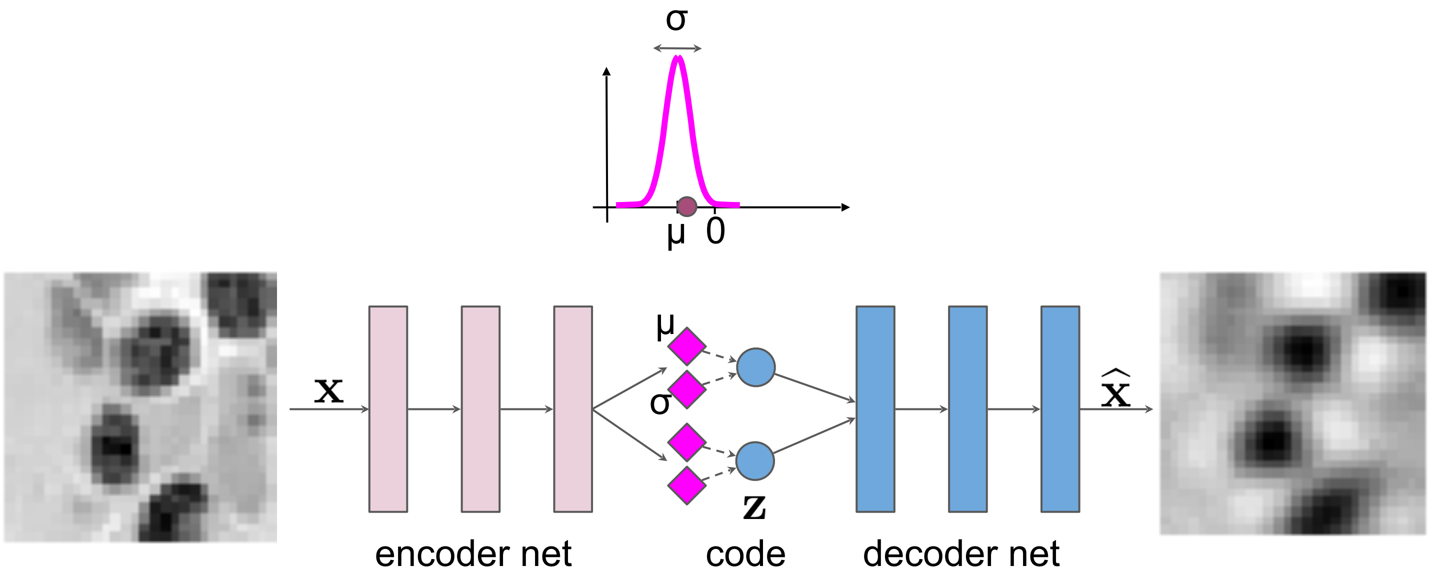
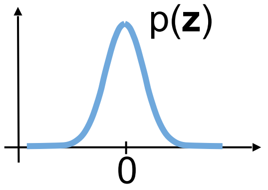
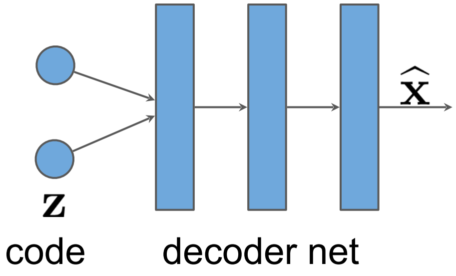


VARIATIONAL AUTO-ENCODERS

VAE has a **marginal** on the latent code.

VAE can **generate** new data.





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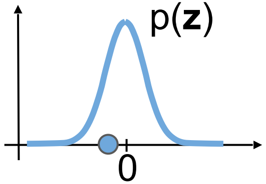

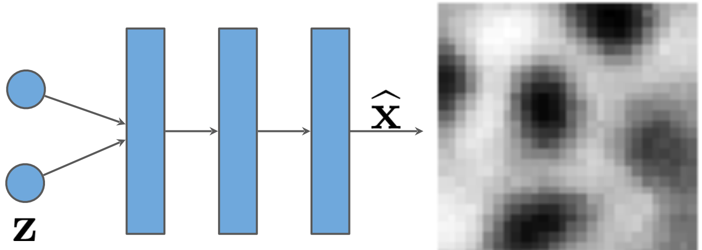

code decoder net

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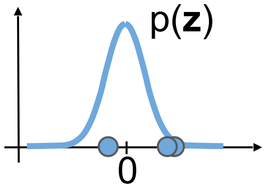

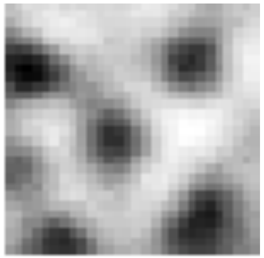

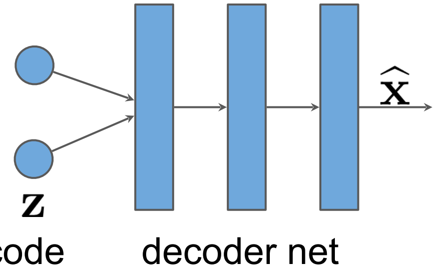

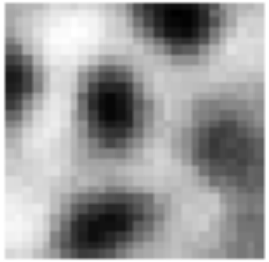

COMMON ISSUES WITH VAES

$$q_\phi(\mathbf{z}|\mathbf{x}) \propto p_\theta(\mathbf{x}|\mathbf{z})\ p_\lambda(\mathbf{z})$$

Weak decoders → bad generations/reconstructions

Weak encoders → bad latent representation

Weak marginals → bad generations

Variational posteriors → what family of distributions?

Others…

COMPONENTS OF VAES

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})$$

Resnets
DRAW
Autoregressive models
Normalizing flows

Autoregressive models
Normalizing flows
VampPrior
Implicit prior

COMPONENTS OF VAES

$$q_{\phi}(\mathbf{z}|\mathbf{x}) \propto p_{\theta}(\mathbf{x}|\mathbf{z})\ p_{\lambda}(\mathbf{z})$$

Normalizing flows
Discrete encoders
Hyperspherical dist.
Hyperbolic-normal dist.
Group theory

Resnets
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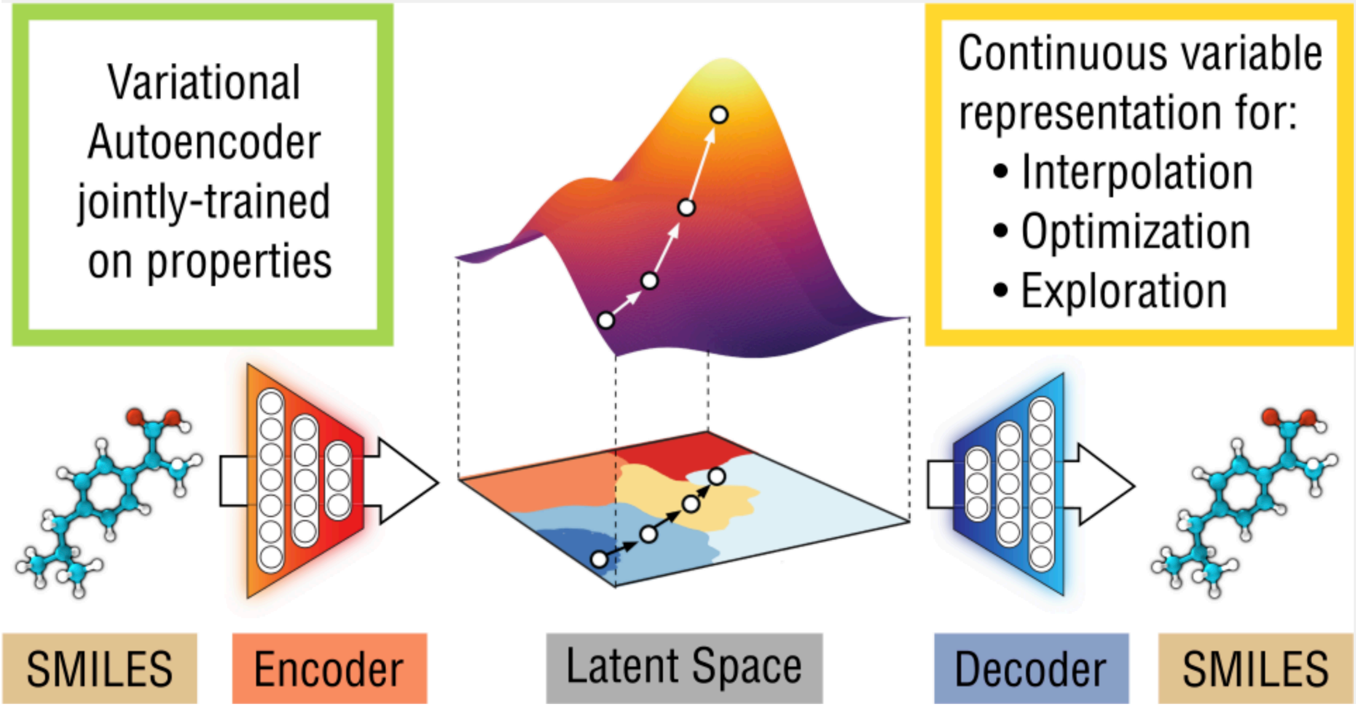
Normalizing flows
VampPrior
Implicit prior

$$\mathrm{ELBO}(\mathbf{x};\theta,\phi,\lambda)$$

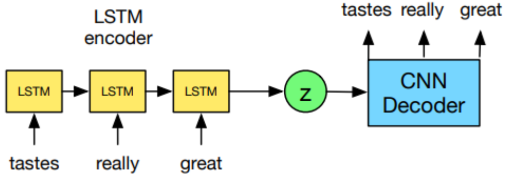
Adversarial learning
MMD
Wasserstein AE

APPLICATIONS

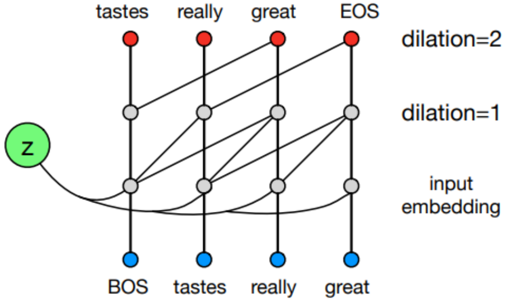


Gómez-Bombarelli, Rafael, et al. "Automatic chemical design using a data-driven continuous representation of molecules." *ACS central science* 4.2 (2018)

APPLICATIONS

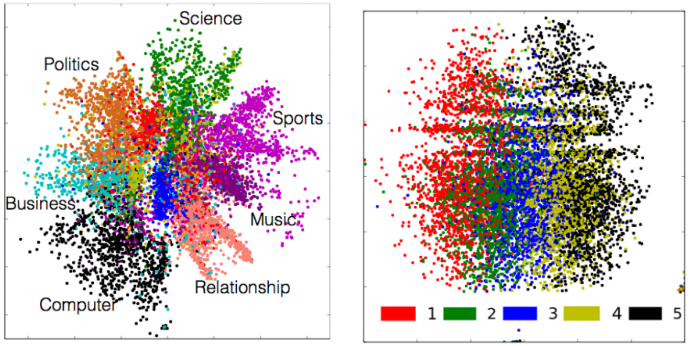


(a) VAE training graph using a dilated CNN decoder.



(b) Digram of dilated CNN decoder.

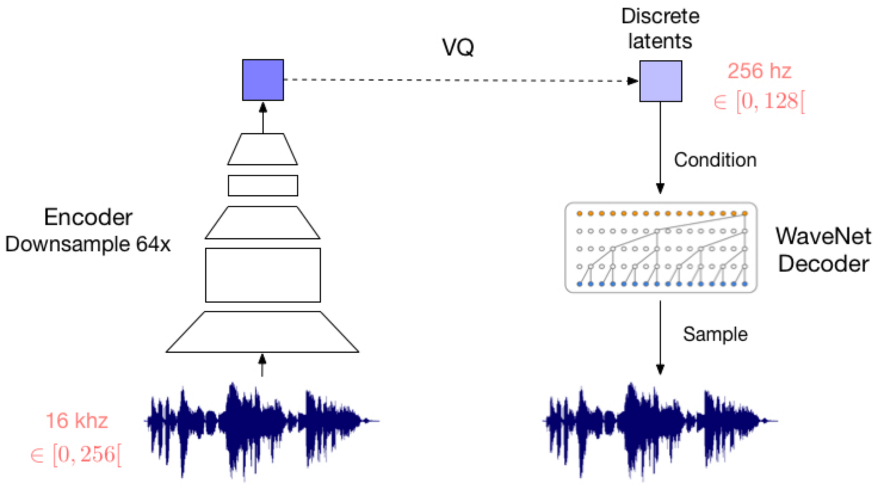
1 star	the food was good but the service was horrible . took forever to get our food . we had to ask twice for our check after we got our food . will not return .
2 star	the food was good , but the service was terrible . took forever to get someone to take our drink order . had to ask 3 times to get the check . food was ok , nothing to write about .
3 star	came here for the first time last night . food was good . service was a little slow . food was just ok .
4 star	food was good , service was a little slow , but the food was pretty good . i had the grilled chicken sandwich and it was really good . will definitely be back !
5 star	food was very good , service was fast and friendly . food was very good as well . will be back !



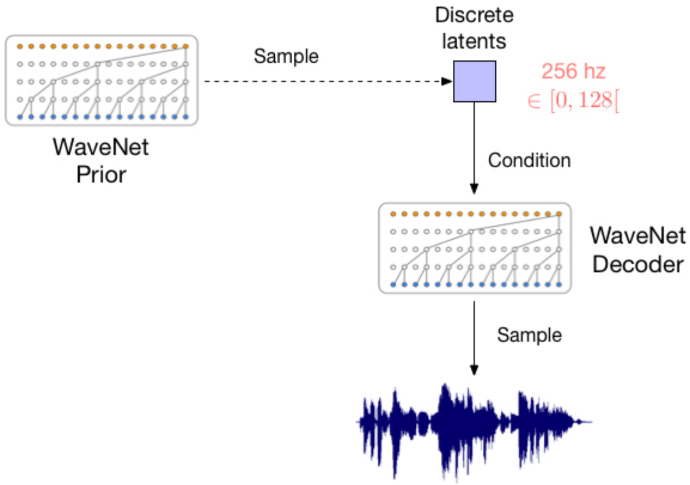
(a) Yahoo (b) Yelp

Yang, Z., Hu, Z., Salakhutdinov, R., & Berg-Kirkpatrick, T. (2017). Improved variational autoencoders for text modeling using dilated convolutions. *ICML 2017*

APPLICATIONS



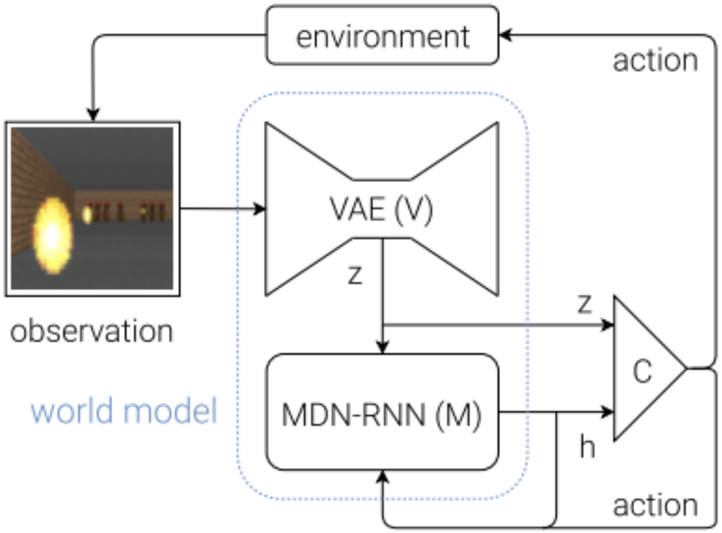
reconstruction

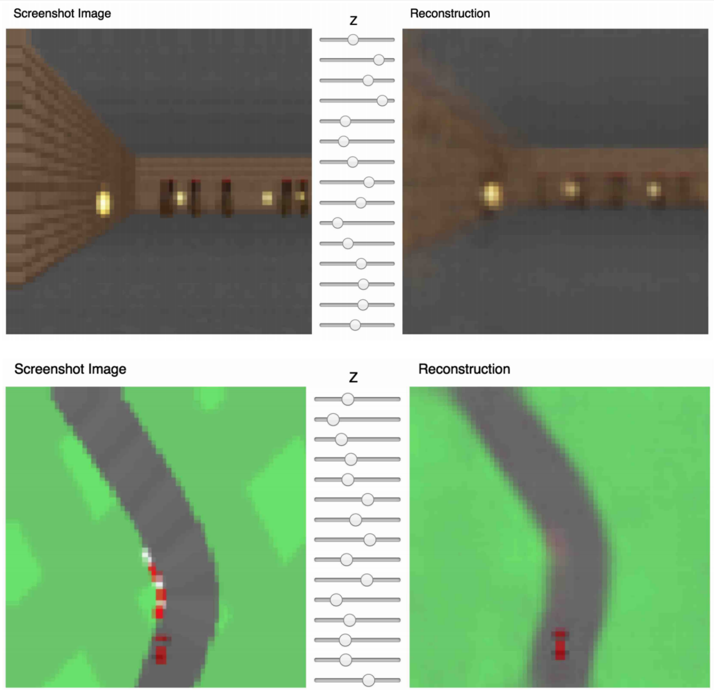


generation

van den Oord, A., & Vinyals, O. (2017). Neural discrete representation learning. *NIPS 2017*.

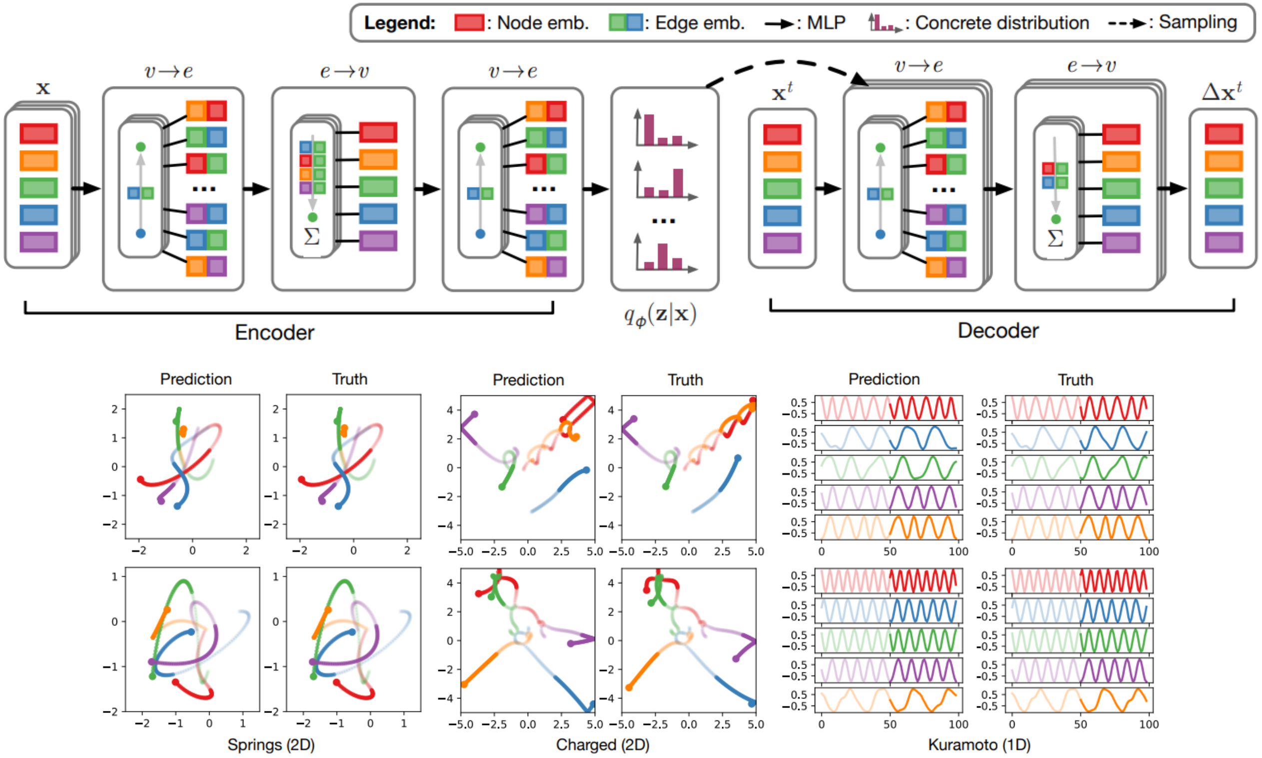
APPLICATIONS





Ha, D., & Schmidhuber, J. (2018). World models. arXiv preprint. *arXiv preprint arXiv:1803.10122*.

APPLICATIONS



Kipf, T., Fetaya, E., Wang, K. C., Welling, M., & Zemel, R. (2018). Neural relational inference for interacting systems. *ICML 2018*.

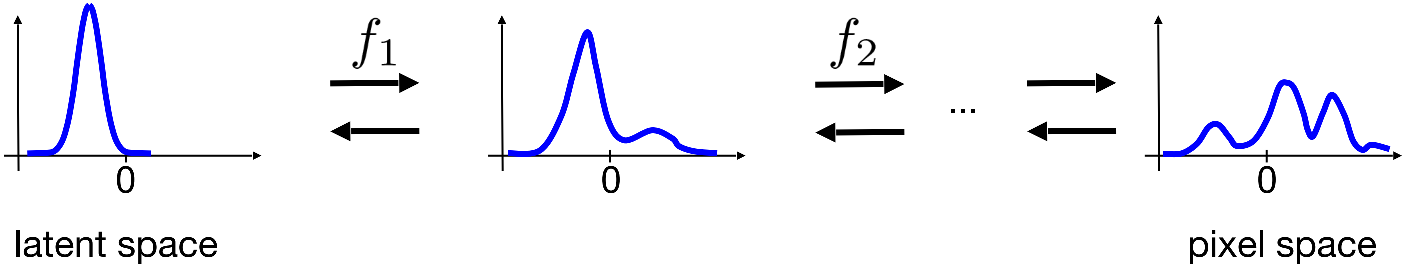
Flow-based models

THE CHANGE OF VARIABLES FORMULA

Let's recall the change of variables formula with invertible transformations:

$$p(\mathbf{x}) = \pi_0\left(\mathbf{z}_0\right) \prod_{i=1}^{K} \left| \det \frac{\partial f_i(\mathbf{z}_{i-1})}{\partial \mathbf{z}_{i-1}} \right|^{-1}$$

We can think of it as an invertible neural network:



Rippel, O., & Adams, R. P. (2013). High-dimensional probability estimation with deep density models. arXiv preprint arXiv:1302.5125.

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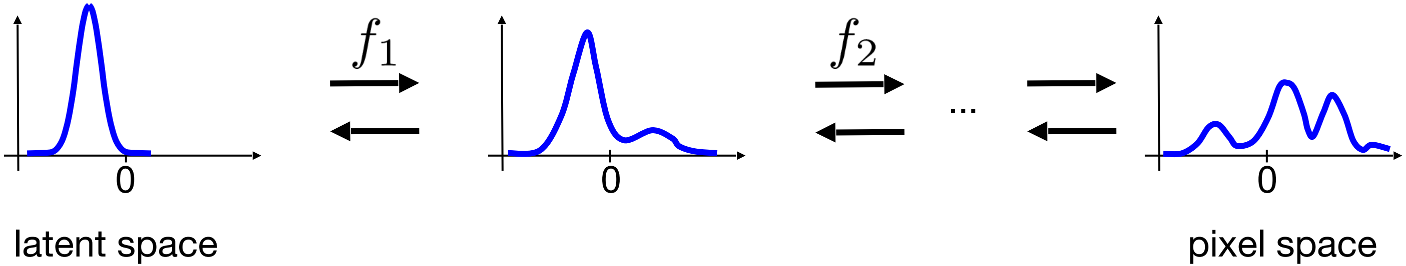

Rippel, O., & Adams, R. P. (2013). High-dimensional probability estimation with deep density models. arXiv preprint arXiv:1302.5125.

REALNVP

Design the invertible transformations as follows:

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d}$$

$$\mathbf{y}_{d+1:D} = \mathbf{x}_{d+1:D} \odot \exp\left(s\left(\mathbf{x}_{1:d}\right)\right) + t\left(\mathbf{x}_{1:d}\right)$$

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. arXiv preprint arXiv:1605.08803.

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Invertible by design:

$$\begin{cases} \mathbf{y}_{1:d} & = \mathbf{x}_{1:d} \\ \mathbf{y}_{d+1:D} & = \mathbf{x}_{d+1:D} \odot \exp\left(s\left(\mathbf{x}_{1:d}\right)\right) + t\left(\mathbf{x}_{1:d}\right) \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}_{1:d} & = \mathbf{y}_{1:d} \\ \mathbf{x}_{d+1:D} & = \left(\mathbf{y}_{d+1:D} - t\left(\mathbf{y}_{1:d}\right)\right) \odot \exp\left(-s\left(\mathbf{y}_{1:d}\right)\right) \end{cases}$$

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Easy Jacobian:

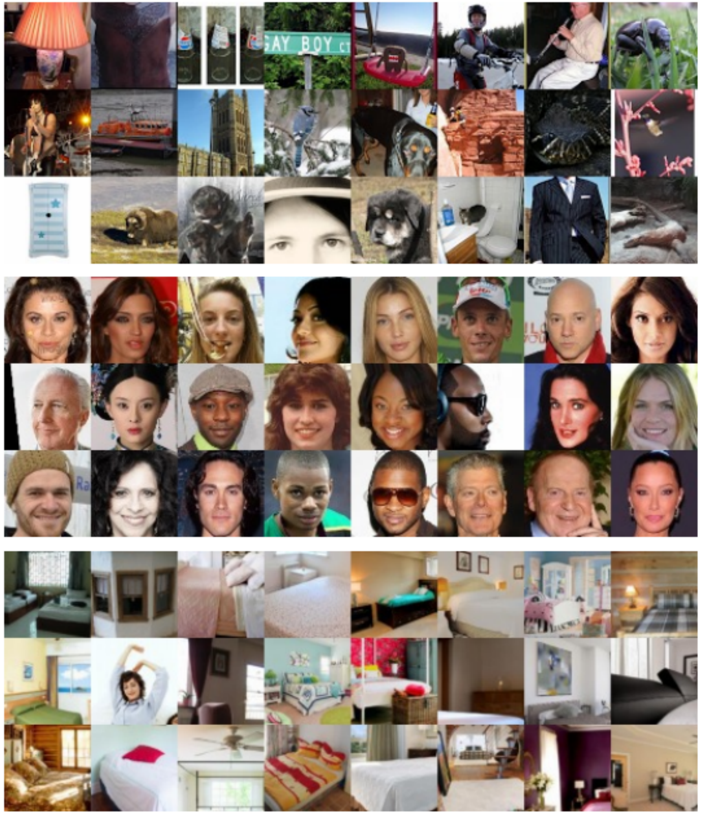
$$\mathbf{J} = \begin{bmatrix} \mathbb{I}_d & \mathbf{0}_{d\times(D-d)} \\ \frac{\partial \mathbf{y}_{d+1:D}}{\partial \mathbf{x}_{1:d}} & \operatorname{diag}\left(\exp\left(s\left(\mathbf{x}_{1:d}\right)\right)\right) \end{bmatrix}$$

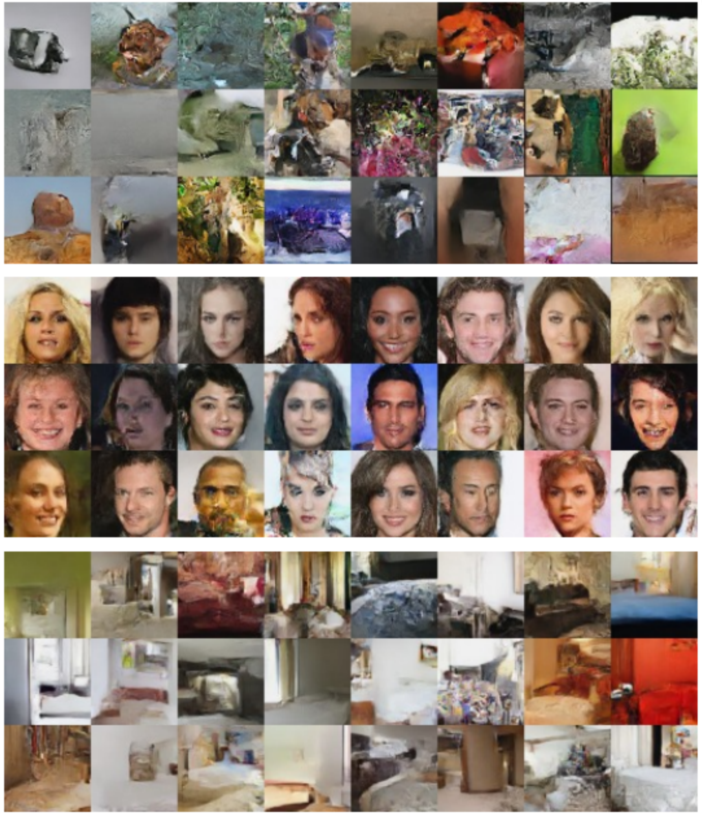
$$\det(\mathbf{J}) = \prod_{j=1}^{D-d} \exp\left(s\left(\mathbf{x}_{1:d}\right)\right)_j = \exp\left(\sum_{j=1}^{D-d} s\left(\mathbf{x}_{1:d}\right)_j\right)$$

Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2016). Density estimation using real nvp. arXiv preprint arXiv:1605.08803.

RESULTS

RESULTS

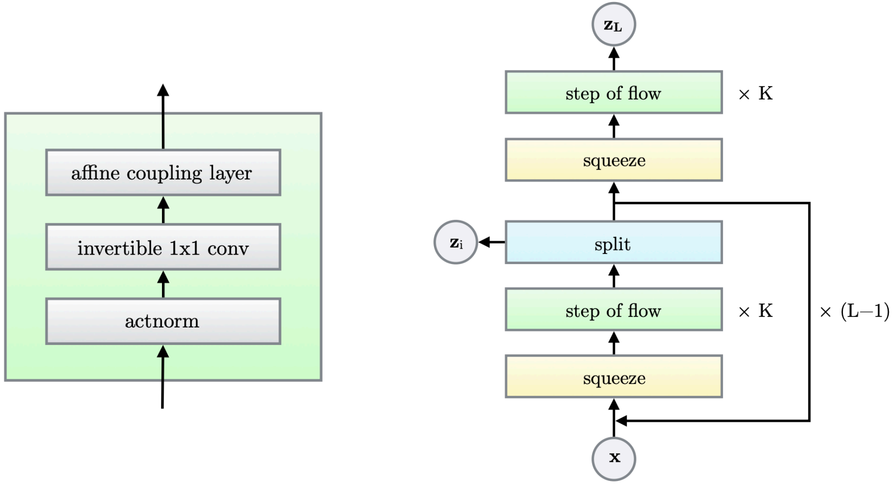




GLOW: REALNVP WITH 1X1 CONVOLUTIONS

A model contains ~1000 convolutions.

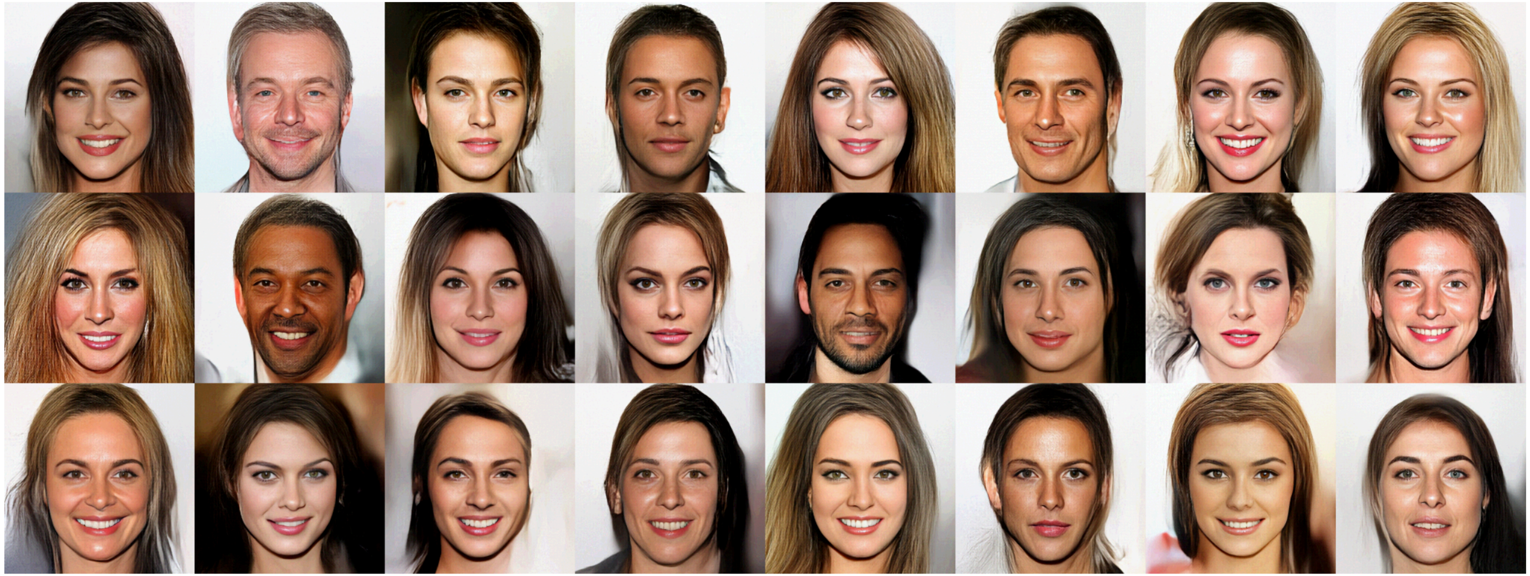
A new component: 1x1 convolution instead of a permutation matrix.



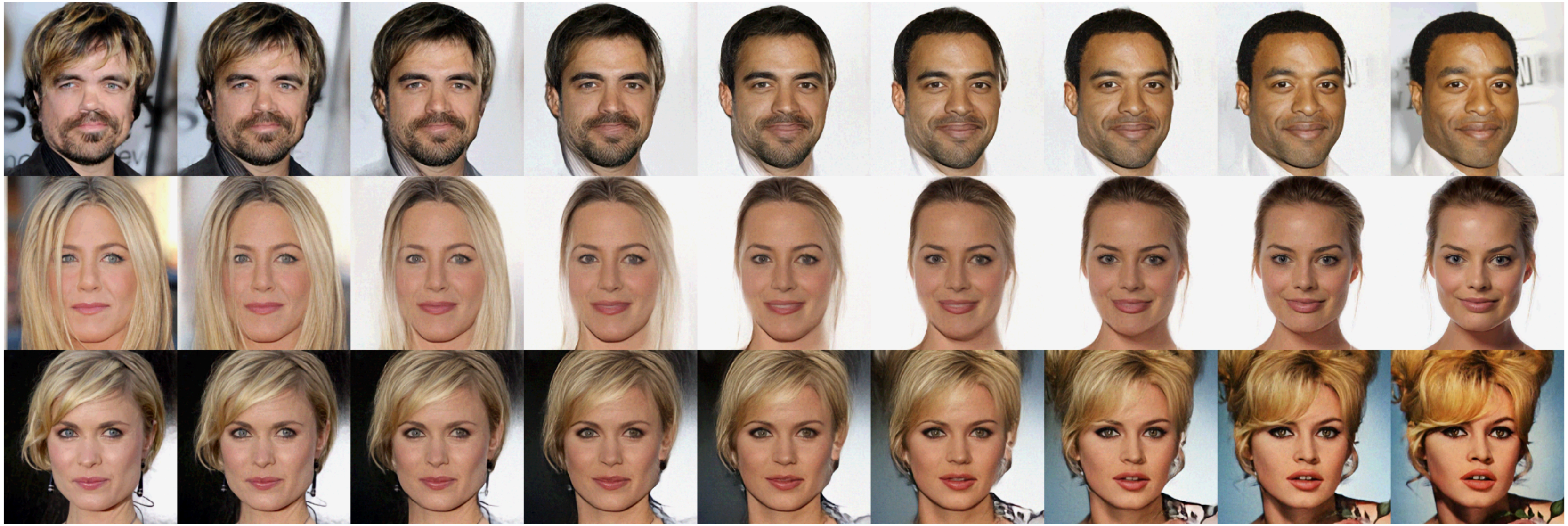
(a) One step of our flow. (b) Multi-scale architecture (Dinh et al., 2016).

Kingma, D. P., & Dhariwal, P. (2018). Glow: Generative flow with invertible 1x1 convolutions. *NeurIPS 2018*

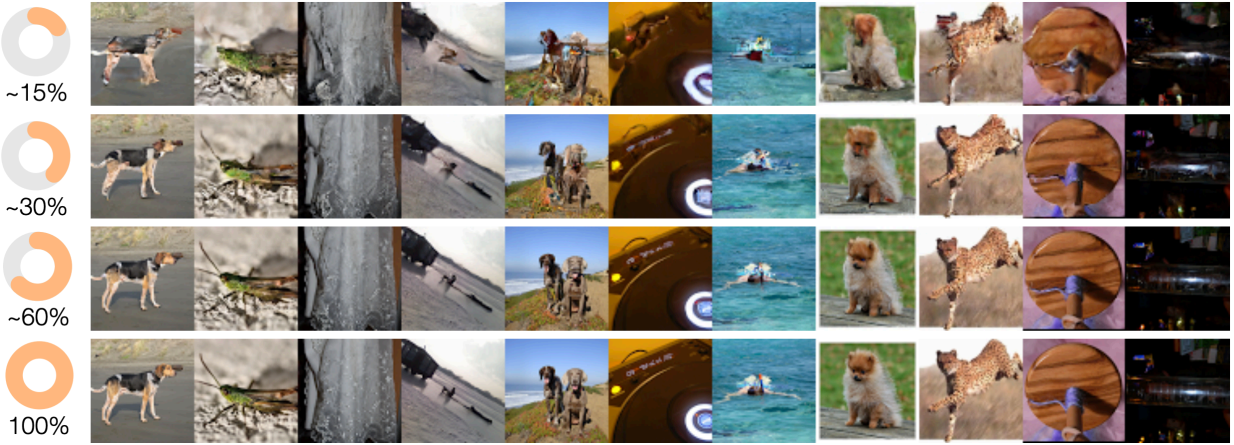
GLOW: SAMPLES



GLOW: LATENT INTERPOLATION



INTEGER DISCRETE FLOW: NO NEED TO CALCULATE JACOBIAN!



Hoogeboom, E., Peters, J. W., Berg, R. V. D., & Welling, M. (2019). Integer Discrete Flows and Lossless Compression. *NeurIPS 2019*

Future directions

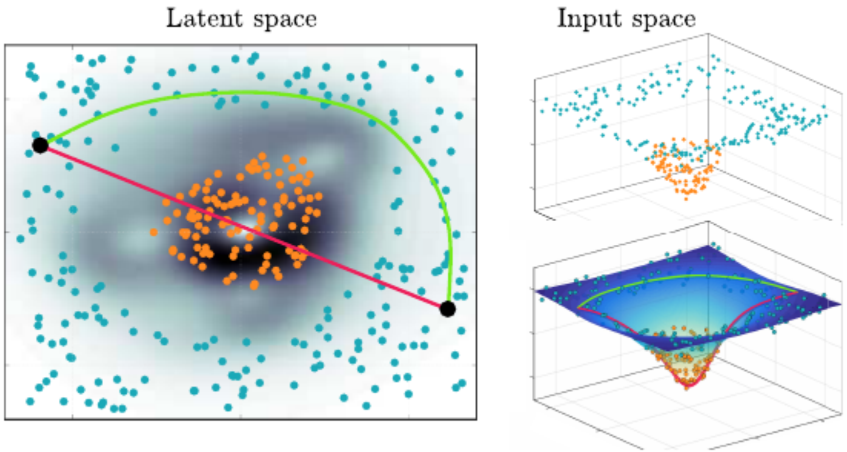
BLURRINESS AND SAMPLING IN VAES

How to avoid sampling from **holes**?

Should we follow **geodesics in the latent space**?

How to use **geometry** of the latent space to build better **decoders**?

How to build **temporal decoders**?



VU

COMPRESSION AND VAES

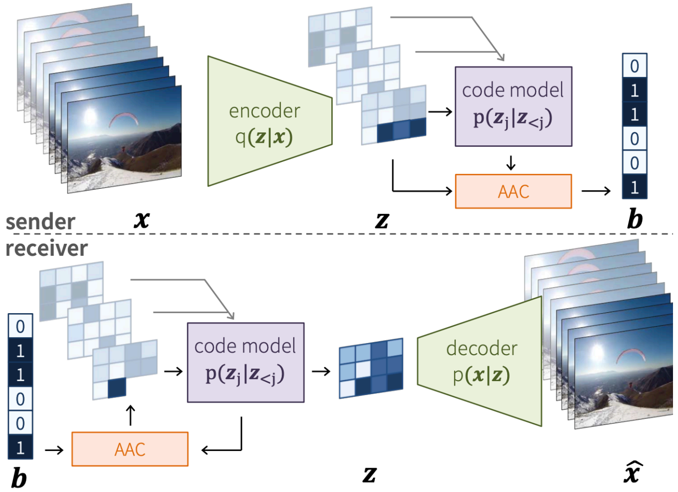
Taking a **deterministic & discrete encoder** allows to simplify the objective.

$$\mathrm{RE}(x|z) - \mathrm{H}[q(z|x)] - \mathrm{CE}[q(z)||p(z)]$$
$$= \mathrm{RE}(x|z) - \mathrm{CE}[q(z)||p(z)]$$

It is important to learn a **powerful prior**. This is challenging!

Is it **easier** to learn a prior with **temporal dependencies**?

Can we alleviate some dependencies by using **hypernets**?



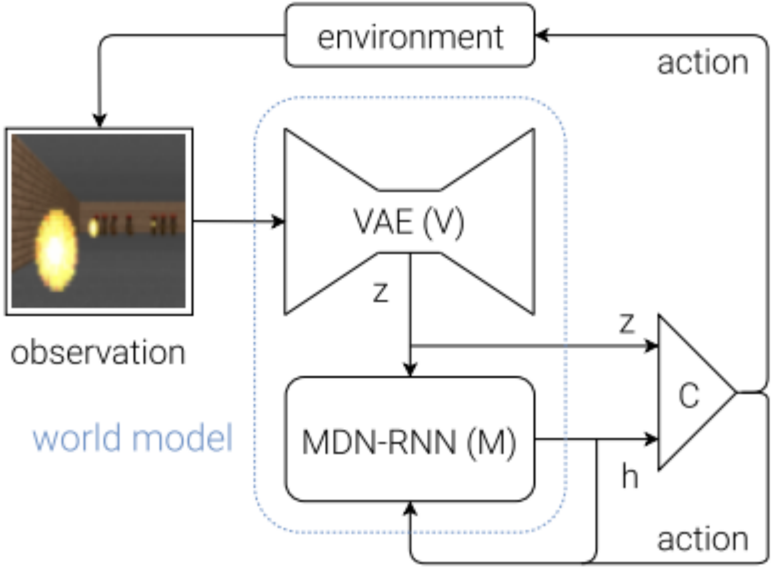
Habibian, A., van Rozendaal, T., Tomczak, J.M., & Cohen, T.S. (2019), Video Compression with Rate-Distortion Autoencoders, ICCV 2019

ACTIVE LEARNING/RL AND VAES

Using **latent representation** to navigate and/or quantify uncertainty.

Formulating **policies** in the latent space entirely.

Do we need a better notion of **sequential dependencies**?



Ha, D., & Schmidhuber, J. (2018). World models. *arXiv preprint arXiv:1803.10122*.

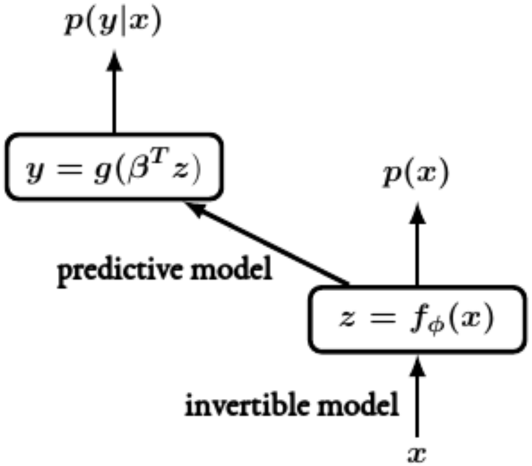
HYBRID AND FLOW-BASED MODELS

We need a **better understanding** of the latent space.

Joining an **invertible model** (flow-based model) with a **predictive model**.

Isn't this model an **overkill**?

How would it work in the **multi-modal learning** scenario?



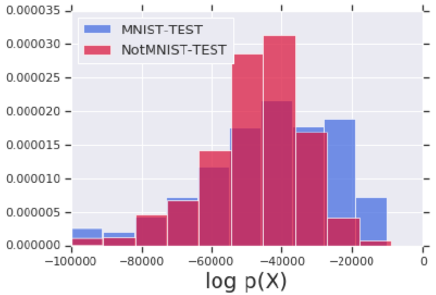
Nalisnick, E., et al. (2019). Hybrid models with deep and invertible features. *arXiv preprint arXiv:1902.02767*.

HYBRID MODELS AND OOD SAMPLE

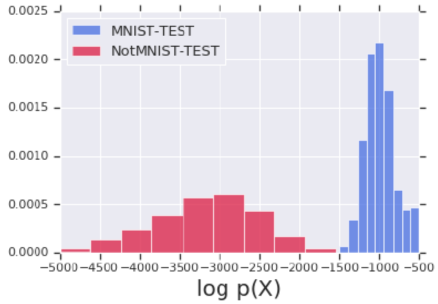
Going back to first slides, we need a good notion of **p(x)**.

Distinguishing **out-of-distribution (OOD)** samples is very important.

Crucial for **decision making**, **outlier detection**, **policy learning**…



(a) Discriminative Model ($\lambda = 0$)



(b) Hybrid Model

Nalisnick, Eric, et al. "Hybrid models with deep and invertible features." *arXiv preprint arXiv:1902.02767* (2019).

Thank you!

Webpage:

https://jmtomczak.github.io/

Code on github:

https://github.com/jmtomczak/

Contact:

jmk.tomczak@gmail.com